Electric-field dependence of acceptor-level binding energies in strained SiGe and InGaAs quantum-well structures

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The acceptor energies for strained SiGe (on Si) and InGaAs (on GaAs) quantum wells are calculated from a 4×4 **k·p** band structure that includes the effects of strain and electric fields. Both center- and edge-doped cases are examined. The theory shows marked changes in the acceptor energies with both strain and electric field. The wide variation in binding energy for the edge-doped quantum wells may provide a mechanism for tunable far-infrared detectors.

Coherently strained quantum-well structures have become important tools for high-performance electronic and optoelectronic devices. Although pseudomorphic structures have been used in III-V systems for a number of years, SiGe alloys grown on Si have only recently received attention. The possibility of introducing strained heterostructure concepts in Si technology is extremely appealing. One of the reasons for the interest in pseudomorphic structures is that the biaxial strain can produce large changes in the valence-band structure. Such changes have important consequences for the hole transport[1] and for the acceptor-level energies.[2–7] So far there have been no theoretical or experimental studies on the acceptor-level energies in the SiGe system. This information is quite important since SiGe is often used as a *p*-type base in Si/SiGe/Si heterojunction bipolar transistors (HBTs). In this communication we present results on the electric-field dependence of strained SiGe and InGaAs quantum-well structures. We see significant changes in the acceptor-level energies as the strain or electric field in the well is varied.

To calculate the acceptor binding energies in quantum wells in presence of strain and transverse electric fields, we start with a description of the valence bands. We represent the valence-band structure by the 4×4 **k·p** (Kohn–Luttinger) Hamiltonian which is valid for systems with large split-off band gaps.[8] This Hamiltonian includes the mixing between the $|\frac{3}{2}, \pm\frac{3}{2}\rangle$ heavy-hole (HH) and $|\frac{3}{2}, \pm\frac{1}{2}\rangle$ light-hole (LH) states. The effect of strain is incorporated via a splitting δ between the light- and heavy-hole diagonal elements. For the $In_yGa_{1-y}As$ (on GaAs) and $Si_{1-x}Ge_x$ (on Si) systems it is approximately given (in eV) by $\delta = -6\epsilon$, where ϵ is the lattice mismatch between the well and the barrier.[9] We assume that the compressive strain is completely absorbed within the well region. In this case, the lattice mismatch ϵ is related to the indium mole fraction y by $\epsilon = -(0.07)y$ and to the germanium mole fraction x by $\epsilon = -(0.04)x$. We obtain the band gap of strained $In_yGa_{1-y}As$ and $Si_{1-x}Ge_x$ from a scaled tight binding model.[10] We assume a valence-band discontinuity of 40% for InGaAs and 90% for SiGe.

Since compressive strain also increases the split-off band gap,[11] we restrict ourselves to large ($x \geq 0.20$) strain values in the $Si_{1-x}Ge_x$ system in order to decouple the four topmost bands from the split-off band. Hence, in the large strain regime the top of the SiGe valence band can be accurately described by the 4×4 **k·p** Hamiltonian.

The effects of an external electric field E are modeled by introducing a diagonal potential eEz common to all terms. We solve for the hole wave functions Ψ_h and energies by discretizing the differential equation into a finite-difference form and diagonalizing the resultant matrix;[12] Ref. 12 describes the effects of strain and electric fields on the hole band structure.

We solve for the acceptor states by directly diagonalizing the Coulomb potential for an impurity located at (x_i, y_i, z_i),

$$V(x,y,z) = (-e^2/\epsilon_r)[(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2]^{-1/2} \quad (1)$$

between the field/strain-dependent basis states Ψ_h. We use a nonvariational discretization technique carried out in **k** space.[6] It should be remarked that the approximations used in Ref. 6 introduce a small splitting of the spin degeneracy which is unphysical.[12,13] We remove this problem by a simple averaging over the spin states.

Since the impurity is in the quantum well with confined hole states, the interaction between the ionized acceptor and the hole state depends upon the position of the acceptor. We will therefore examine two extreme cases. In the first case the acceptor is at the center of the quantum well, while in the second case it is at the edge of the well. Clearly, the binding energy is much smaller for the edge doping case.

In Fig. 1 we show our results for an $In_yGa_{1-y}As/Al_{0.3}Ga_{0.7}As$ quantum well with a 100-Å well size. Two cases are shown, the first one being without any addition of In and the second where 20% excess In is added. If the growth is pseudomorphic, this excess In introduces a 1.4% compressive strain in the plane of the growth. If the strain is relaxed through dislocation formation, however, the results for the InGaAs well are essentially the same as those for the unstrained GaAs well. We

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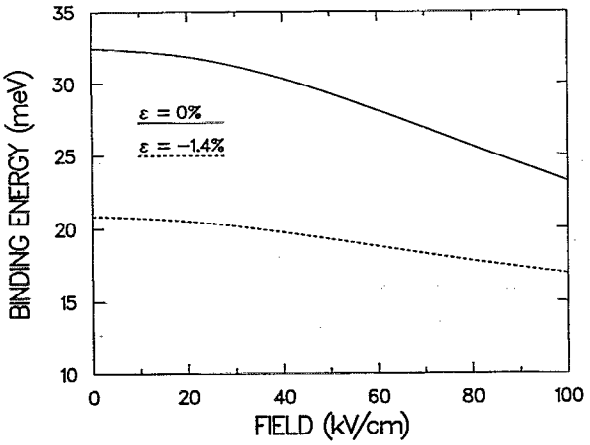

FIG. 1. Lowest-energy center-doped acceptor level as a function of applied electric field in a 100-Å $In_yGa_{1-y}As/Al_{0.3}Ga_{0.7}As$ quantum well. Curves are shown for $\epsilon = 0\%$ and $\epsilon = -1.4\%$.

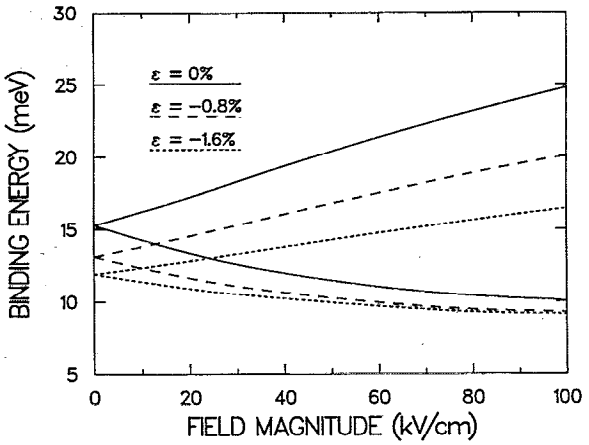

FIG. 3. Lowest-energy edge-doped acceptor level as a function of applied electric-field magnitude in a 100-Å $Si_{1-x}Ge_x/Si$ quantum well. Curves are shown for $\epsilon = 0\%$, $\epsilon = -0.8\%$, and $\epsilon = -1.6\%$.

see that the acceptor-level energies decrease as the electric field increases, since the hole wave functions are pushed toward the edge of the quantum well (away from the Coulomb potential) and are less influenced by the impurity. We also know from simple considerations that a heavier-particle envelope function will shift more rapidly with electric field than a lighter-mass envelope function. It is well known that the unstrained hole masses are much heavier than the strained-well hole masses, and the calculated acceptor energies reflect this behavior. Figure 2 shows similar results for the SiGe/Si quantum-well structures. The curves with $\epsilon = 0$ correspond to relaxed (unstrained) SiGe well material confined by Si barriers. We see that the effects are similar to those manifested in the InGaAs structures.

In Fig. 3 we show the results for the SiGe/Si system with the dopant at the edge of the quantum well. In this case the acceptor-level energies are dependent upon the polarity of the transverse electric field. In one electric-field orientation the hole states are pushed away from the dopant, while in the opposite orientation the hole states are pulled closer to the impurity. Hence, the acceptor-level energies either increase or decrease with the applied field. The starting value of the acceptor-level energy is small compared to the center-doped case, but can be seen to increase to a very large value for one of the transverse field orientations. The wide energy-level variation (~ 15 meV) available may be useful for producing tunable far-infrared detectors.

In summary, we have examined the effect of electric fields and strain on the acceptor levels in SiGe/Si and InGaAs/AlGaAs quantum wells. The acceptor-level energies decrease as the strain is increased. They also show a decrease with electric field for the center-doped case. For the edge-doped case we see that the acceptor-level energies are dependent on the field direction, increasing in one direction and decreasing in the other.

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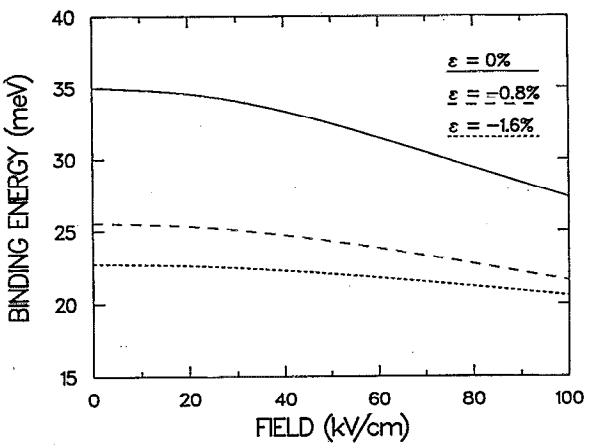

FIG. 2. Lowest-energy center-doped acceptor level as a function of applied electric field in a 100-Å $Si_{1-x}Ge_x/Si$ quantum well. Curves are shown for $\epsilon = 0\%$, $\epsilon = -0.8\%$, and $\epsilon = -1.6\%$.

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